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ALE3D Statistical Hot Spot Model Results for LX-17

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ALE3D STATISTICAL HOT SPOT MODEL RESULTS FOR LX-17

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The Statistical Hot Spot shock initiation and detonation reactive flow model for solid explosives in the ALE3D hydrodynamic computer code provides physically realistic descriptions of: hot spot formation; ignition (or failure to ignite); growth of reaction (or failure to grow) into surrounding particles; coalescence of reacting hot spots; transition to detonation; and self-sustaining detonation. The model has already successfully modeled several processes in HMX-based explosives, such as shock desensitization, that can not predicted by other reactive flow models. In this paper, the Statistical Hot Spot model is applied to experimental embedded gauge data on the insensitive triaminotrintrobenzene (TATB) based explosive LX-17.

INTRODUCTION

The Statistical Hot Spot reactive flow model (1) was formulated in the ALE3D hydrodynamic code (2) to provide physically realistic descriptions of "hot spot" ignition, growth and coalescence. The details of its mathematics and material models were discussed previously (1), along with applications to HMX-based explosives. Besides shock initiation and detonation properties that the Ignition and Growth model (3) predicts, the Statistical Hot Spot model successfully calculated shock desensitization results (4) on PBX 9404 (94% HMX, 3% nitrocellulose, 3% CEF) that no other model has simulated. In this paper, the Statistical Hot Spot model is applied to the insensitive high explosive LX-17 (92.5% TATB and 7.5% KelF binder at 98% theoretical density).

The alternating amino and nitro groups on TATB's benzene ringlead to strong intra- and inter-molecular hydrogen bonding. This hydrogen bonding is a major factor in TATB's high activation energy for thermal decomposition (60 kcal/mol, compared to 40 – 50 kcal/mol for other explosives) (5). Hydrogen bonding also contributes to the high thermal diffusivity of TATB, which is 1.6 to 3 times that of other explosives (6). This high thermal diffusivity causes shock induced "hot spots" to cool before they can react and grow (7). LX-17 requires sustained shock pressures of 6.5 GPa to cause any reaction. An 8.4 GPa sustained shock pressure in LX-17 causes slow growth of hot spots (8). Once ignited, LX-17 deflagrates an order of magnitude more slowly than other solid explosives. Under extremely high pressures in a diamond anvil cell, TATB deflagrates at rates less than 22 m/s (9), whereas HMX deflagrates at rates approaching 1000 m/s (10). Due to the slow growth rates of spreading hot spots, the shock to detonation transition in LX-17 takes longer than other explosives (11). The reaction zone length of fully detonating LX-17 is 3 mm, which causes detonation wave curvature (12). TATB reactive flow models must reproduce this insensitivity.

NEW MODEL IMPROVEMENTS

In the previous version of the model(1), a second order accurate pressure, temperature equilibration scheme was used to the close the explosive mixture equation of state. In this version, a self-consistent second order accurate pressure equilibration with non-equilibrium temperatures is used. The temperature is determined by tracking the flow of energy from reactant to product states. The pressure dependent change in composition at each time step is determined self-consistently using an average of the initial and final pressures. The final state volumes are adjusted by iteration until the errors in pressure and composition reach acceptable levels.

LX-17 MODEL PARAMETERS

The Statistical Hot Spot model requires an unreacted equation of state, a reaction product equation of state, and a set of 8 reaction rate parameters: P_0, P^*, A, μ, ν, D, ρ_P^0, and ε (1). The unreacted equation of state is the Jones-Wilkins-Lee (JWL) fit used in the Ignition and Growth model (12). The reaction products are described by LEOS tables calculated by the CHEETAH code (13). P_0 is the ignition rate threshold pressure at which pores collapse and is related to the yield strength. P* is the saturation pressure at which all potential hot spots have been created. A is the ignition pre-factor, which is related to the reacting surface area. μ and D are the hot spot death rate and constant death rate parameter, respectively. D is related to the shock pressure at which the explosive begins to ignite. The deflagration velocity ν can be experimentally determined in diamond anvil experiments (9,10). ρ_P^0 is initial number of hot spot sites, and ε is the initial hot spot diameter. The seven constant reaction rate parameters for LX-17 are listed in Table 1, along with those used for HMX. Table 2 lists the assumed dependence of ν as a function of pressure for LX-17 and HMX. Tables 1 and 2 show that the reaction rates for LX-17 are much slower and the LX-17 hot spots die out more completely than those of HMX. The saturation pressure P_0 for LX-17 is set to 15 GPa, whereas 10 GPa was used for HMX.

Table 1. Reaction Rate Parameters

Parameter	HMX Value	LX-17 Value
P_0	0.1 GPa	0.1 GPa
P*	10 GPa	15 GPa
A	2000 cm-μs/g	1000 cm-μs/g
μ	5 μs^{-1}	10 μs^{-1}
D	11.3	30
ρ_P^0	1.4 x 10^{10} cm^{-3}	1.4 x 10^{10} cm^{-3}
ε	1.5 x 10^{-4} cm	1.5 x 10^{-5} cm

Table 2. Deflagration Speed ν vs Pressure

Pressure(GPa)	HMX ν(cm/μs)	LX17(cm/μs)
0.0001	$2.35x10^{-7}$	$2.35x10^{-7}$
0.1	$5x10^{-5}$	$5x10^{-5}$
3	$7x10^{-4}$	$4x10^{-4}$
12	$3x10^{-2}$	$2x10^{-3}$
50	$9x10^{-2}$	$4x10^{-3}$

LX-17 MODELING RESULTS

The first test of the LX-17 model is shock initiation caused by driving the explosive into a stone wall at various initial velocities. Figure 1 shows the pressure contours after 7 μs of propagation following a 0.7 km/s impact. This initial shock pressure is approximately 6.5 GPa, which induces very little reaction in LX-17. The maximum shock pressure has decreased to 4.6 GPa in Fig. 1. Figure 2 shows the fraction reacted contours for the same time. The maximum fraction

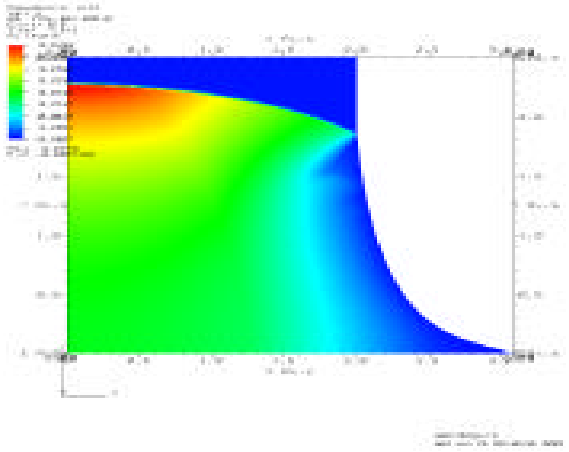

FIGURE 1. Pressure contours in LX-17 impacted into a stone wall at 0.7 km/s after 7 μs of propagation

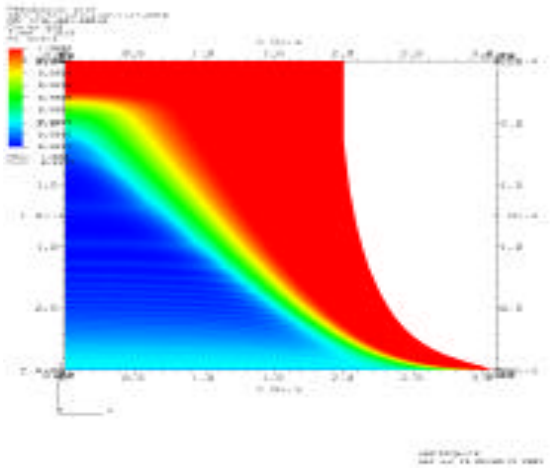

FIGURE 2. Fraction reacted contours for LX-17 7 μs after collision with a stone wall at 0.7 km/s

is 0.6%, which agrees with experiments at 6.5 GPa. Figure 3 shows the pressure contours in LX-17 3.9 ms after impact with a stone wall at 1.8 km/s. the pressure has reached 34 GPa, the von Neumann spike value for LX-17 detonation. Figure 4 shows the corresponding fraction reacted contours, which show a maximum of over 90% reacted as this wave builds to steady detonation. At steady state detonation, the calculated detonation velocity agrees closely with the experimental value of 7.6 mm/μs. Thus the LX-17 model predictions agree well with single shock initiation and detonation experiments.

Another test for the LX-17 model is the series of 12 reflected shock experiments reported by Tarver et al. (14). LX-17 was subjected to impact shock

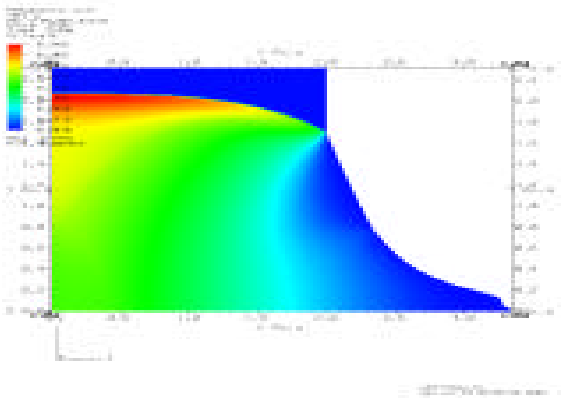

FIGURE 3. Pressure contours in LX-17 3.9 μs after impact with a stone wall at 1.8 mm/μs

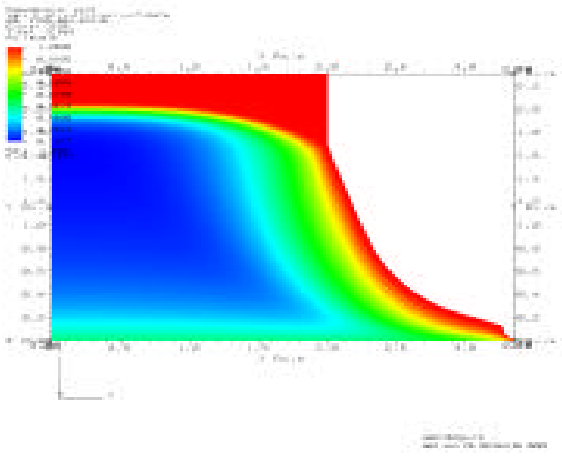

FIGURE 4. Fraction reacted contours for LX-17 3.9 μs after impact with a stone wall at 1.8 mm/μs

pressures of 4.4 GPa to 8.6 GPa, and then these shocks were reflected back into the LX-17 off aluminum, copper, or tantalum dics. The lowest pressure shocks caused desensitization, or "dead pressing," while higher pressures caused partial reactions behing the front shock and faster reactions or detonation behind the reflected shocks. All 12 experiments were modeled with the Statistical Hot Spot model with good results. Two examples are shown in Figs. 5 – 8. Figure 5 shows pressure contours 6.4 μs after steel flyer impact at 1 km/s and reflection off a copper disc. The impact pressure was 6.8 GPa and the reflected shock pressure was 14 GPa. This shot exhibited shock desensitization on the embedded pressure gauges shown in Fig. 2 of Tarver et al. (14). Figure 6 shows that the LX-17 model predicts this desensitization, because its

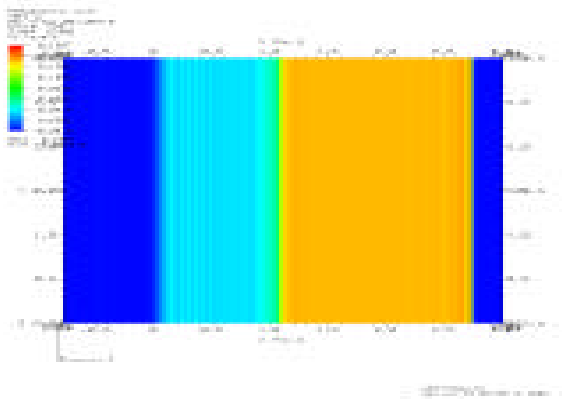

FIGURE 5. Pressure contours in LX-17 6.4 μs after steel flyer impact at 1 km/s and reflection by copper

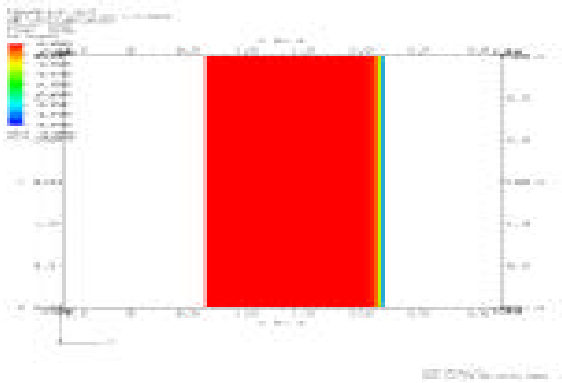

FIGURE 6. Fraction reacted contours in LX-17 6.4 μs after steel impact at 1 km/s and reflection at copper disc

maximum fraction reacted is only 6% at 14 GPa.

Figure 7 contains the LX-17 pressure contours 5 μs after impact by a steel flyer at 1.19 km/s followed by shock reflection off a tantalum disc. The impactpressure is 8.1 GPa, which causes c reaction . The reflected shock pressures in the reacting LX-17 are over 20 GPa, resulting in faster reaction and build up to detonation. Figure 8 shows the fraction reacted contours at 5 μs. The maximum fraction reacted has already reached 40% at the LX-17-Ta boundary and continues to rapidly grow to 100% and produce detonation. The LX-17 parameters simulate the main features of the 12 reflected shock experiments.

SUMMARY

The LX-17Statistical Hot Spot model accurately simulates single and reflected shock initiation data, because it is based on physical descriptions of hot spot ignition, death, growth, and coalescence.

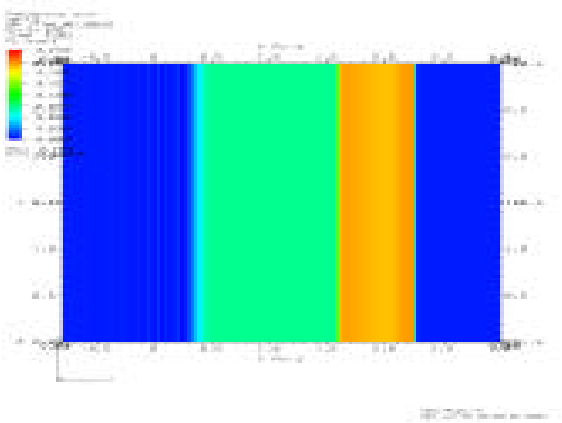

Figure 7. Pressure contours in LX-17 5 μs after steel impact at 1.19 km/s followed by tantalum reflection

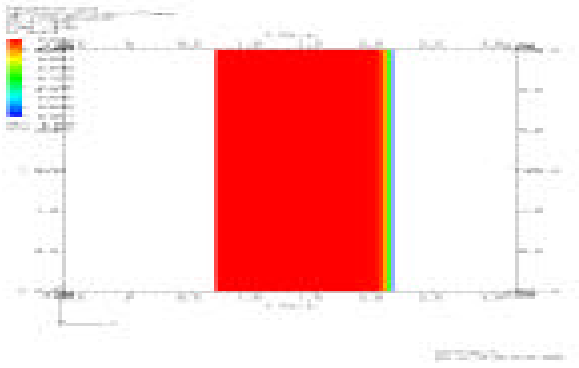

Figure 8. Fraction reacted contours in LX-17 5 μs after steel impact and reflection off a tantalum disc

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